201-16554K

IUCLID

Data Set

Existing Chemical	:	ID: 84-77-5
Memo	:	HPV Chemical
CAS No.	:	84-77-5
TSCA Name	:	1,2-benzenedicarboxylic acid, didecyl ester
Generic name	:	didecyl phthalate
Molecular Formula	:	C28H46O4

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	06.07.2006
Revision date	:	
Date of last update	:	06.07.2006
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
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Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freetext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)

68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :

Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -46 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited information on how the data were developed.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (5)

Value	:	136 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(3) invalid

05.06.2006 (2)

2.2 BOILING POINT

Value	:	477 °C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (2)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.0000000184 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including didecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for didecyl phthalate ester was 609.2 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
05.06.2006		(1)

Value	:	.000000136 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester

Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	9.46 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including didecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for didecyl phthalate ester was 609.2 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (1)

Partition coefficient	:	octanol-water
Log pow	:	10.5 at 25 °C
pH value	:	

Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.0381 other: ug/L at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including didecyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for didecyl phthalate ester was 609.2 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths

from 1 to 13 carbons.

Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (1)

Solubility in	:	Water
Value	:	.00168 other: ug/L at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 6.46.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.00000000002623 cm³/(molecule*sec)
Degradation	:	50 % after 4.9 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 4.89 hrs or 0.41 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

05.06.2006 (2)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	7.7 year at 25 °C
t1/2 pH9	:	- at °C
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPI SuiteTM version 3.12., that is based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used by the US EPA for estimating chemicophysical properties of substances.
Test substance	:	CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on chemical structure as modeled by EPI SuiteTM. This robust summary has a reliability rating of 2 because the

data are calculated and not measured.

Flag : Critical study for SIDS endpoint
06.07.2006 (2)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1997

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model to represent didecyl phthalate ester were:
MW = 446.68
Temperature = 25C
Water Solubility = 0.0000381 mg/L
Vapor Pressure = 0.0000000184 Pa
Pow = 9.46
Melting Point = -46C

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).

Result : Soil = 97.7%
Air = 0.0%
Water = 0.0%
Sediment = 2.2%
Suspended sed. = 0.1%
Biota = 0.0%

Test substance : CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag : Critical study for SIDS endpoint
05.06.2006 (4)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical input values for the model to represent didecyl phthalate

ester were:
MW = 446.68
Temperature = 25C
Water Solubility = 0.0000381 mg/L
Vapor Pressure = 0.0000000184 Pa
Pow = 9.46
Melting Point = -46C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	9.7a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from EBSI (1995) and Boethling (2000): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment).

Result : Using the Mackay Level I calculation, the following distribution is predicted for didecyl phthalate ester:

Compartment	%Distribution
Air	0.9
Water	8.2
Soil	68.4
Sediment	22.5

Test substance : CAS #84-77-5; 1,2-benzenedicarboxylic acid, didecyl ester

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

05.06.2006 (3)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere 41, 1389-1399.

(2) Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.

(3) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.

(4) Mackay D, DiGuardo A, Paterson S and Cowan C (1997). EQC Model ver. 1.01, available from the Environmental Centre, Trent University, Canada.

(5) Staples C, Peterson D, Parkerton T and Adams W (1997). The environmental fate of phthalate esters: A literature review. Chemosphere 35, 667-749.

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

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10.3 RISK ASSESSMENT